

# Preconditioned iterative methods for space-time fractional advection-diffusion equations

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## Abstract

In this paper we want to propose practical numerical methods to solve a class of initial-boundary problem of space-time fractional advection-diffusion equations. To start with, an implicit method based on two-sided Grünwald formulae is proposed with a discussion of the stability and consistency. Then, the preconditioned generalized minimal residual (preconditioned GMRES) method and the preconditioned conjugate gradient normal residual (preconditioned CGNR) method, with an easily constructed preconditioner, are developed. Importantly, because the resulting systems are Toeplitz-like, the fast Fourier transform can be applied to significantly reduce the computational cost. Numerical experiments are implemented to show the efficiency of our preconditioner, even with cases of variable coefficients.

*Keywords:* Fractional diffusion equations; Shifted Grünwald discretization; Toeplitz matrix; Preconditioner; Fast Fourier transform; CGNR method; GMRES method.

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## 1. Introduction

This article is concerned with numerical approaches for solving the initial-boundary value problem of the space-time fractional advection-diffusion equation (STFDE) [1]:

$$\begin{cases} \frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = -d_+(x, t)D_{a,x}^\beta u(x, t) - d_-(x, t)D_{x,b}^\beta u(x, t) + \\ \quad e_+(x, t)D_{a,x}^\gamma u(x, t) + e_-(x, t)D_{x,b}^\gamma u(x, t) + f(x, t), \\ u(x, 0) = \phi(x), \quad a \leq x \leq b, \\ u(a, t) = u(b, t) = 0, \quad 0 < t \leq T, \end{cases} \quad (1)$$

where  $\alpha, \beta \in (0, 1]$ ,  $\gamma \in (1, 2]$ ,  $a < x < b$ , and  $0 < t \leq T$ . Here, the parameters  $\alpha, \beta$  and  $\gamma$  are the order of the STFDE,  $f(x, t)$  is the source term, and diffusion coefficient functions  $d_\pm(x, t)$  and  $e_\pm(x, t)$  are non-negative under the assumption that the flow is from left to right. The STFDE can be regarded as generalizations of classical advection-diffusion equations with the first-order time derivative replaced by the Caputo fractional derivative of order  $\alpha \in (0, 1]$ , and the first-order and the second-order space derivatives replaced by the two-sided Riemann-Liouville fractional derivatives of order  $\beta \in (0, 1]$  and of order  $\gamma \in (1, 2]$ . Namely, the time fractional derivative in (1) is the Caputo fractional derivative of order  $\alpha$  [2] denoted by

$$\frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial u(x, \psi)}{\partial \psi} \frac{d\psi}{(t-\psi)^\alpha}, \quad (2)$$

and the left-handed ( $D_{a,x}^\alpha$ ) and the right-handed ( $D_{x,b}^\alpha$ ) space fractional derivatives in (1) are the Riemann-Liouville fractional derivatives of order  $\alpha$  [2, 3] which are defined by

$$D_{a,x}^\alpha u(x, t) = \frac{1}{\Gamma(m-\alpha)} \frac{\partial^m}{\partial x^m} \int_a^x \frac{u(s, t)}{(x-s)^{\alpha-m+1}} ds, \quad (3a)$$

and

$$D_{x,b}^\alpha u(x, t) = \frac{(-1)^m}{\Gamma(m-\alpha)} \frac{\partial^m}{\partial x^m} \int_x^b \frac{u(s, t)}{(s-x)^{\alpha-m+1}} ds, \quad (3b)$$

where  $\Gamma$  denotes the gamma function, and  $m$  is an integer satisfying  $m-1 < \alpha \leq m$ . Truly, when  $\alpha = \beta = 1$  and  $\gamma = 2$ , the above equation reduces to the classical advection-diffusion equation.

The study of fractional calculus can be traced to late 17th century [4, 3, 5], but it was not until late 20th century that fractional differential equations (FDEs) become important due to its wide applications in finance [6, 7, 3, 8], physics [9, 10, 11, 12, 13, 14, 15], image processing [16], and even biology [17]. Though analytic approaches, such as the Fourier transform method, the Laplace transform methods, and the Mellin transform method, have been proposed to seek closed-form solutions [2], there are very few FDEs whose analytical closed-form solutions are

available. Therefore, the research on numerical approximation and techniques for the solution of FDEs has attracted intensive interest; see [18, 19, 20, 21, 22, 23, 24, 25, 26, 27] and references therein. Importantly, traditional methods for solving FDEs tend to generate full coefficient matrices, which incur computational cost of  $\mathcal{O}(N^3)$  and storage of  $\mathcal{O}(N^2)$  with  $N$  being the number of grid points [27].

To optimize the computational complexity, a shifted Grünwald discretization scheme with the property of unconditional stability was proposed by Meerschaet and Tadjeran [21, 22] to approximate the FDE. Later, Wang *et al.* [27] discovered that the linear system generated by this discretization has a special Toeplitz-like coefficient matrix, or, more precisely, this coefficient matrix can be expressed as a sum of diagonal-multiply-Toeplitz matrices. This implies that the storage requirement is  $\mathcal{O}(N)$  instead of  $\mathcal{O}(N^2)$ , and the complexity of the matrix-vector multiplication only requires  $\mathcal{O}(N \log N)$  operations by the fast Fourier transform (FFT) [28, 29, 30]. Upon using this advantage, Wang *et al.* proposed the CGNR method having computational cost of  $\mathcal{O}(N \log^2 N)$  to solve the linear system and numerical experiments show that the CGNR method is fast when the diffusion coefficients are very small, i.e., the discretized systems are well-conditioned [31].

However, the discretized systems become ill-conditioned when the diffusion coefficients are not small. In this case, the CGNR method converges slowly. To overcome this shortcoming, preconditioning techniques have been introduced to improve the efficiency of the CG method with the total complexity being  $\mathcal{O}(N \log N)$  operations at each time step [32, 33]. For the same reason, we propose two preconditioned iterative methods, i.e., the preconditioned GMRES method and the preconditioned CGNR method, and observe results related to the acceleration of the convergence of the iterative methods, while solving (1).

This paper is organized as follows. In section 2, we give an implicit difference method for (1) and prove that this scheme is unconditionally stable, convergent and uniquely solvable. In section 3, we propose the preconditioned GMRES method and the preconditioned CGNR method to solve (1) by exploring the matrix representation of the implicit difference scheme. Finally, we present numerical experiments to show the efficiency of our numerical approaches in section 4 and provide concluding remarks in section 5.

## 2. Implicit difference method

In this section, we present an implicit difference method for solving (1) by discretizing the STFDE defined by (1). Unlike the approach given by Liu *et al.* in [1], we use henceforth two-sided fractional derivatives to approximate the Riemann-Liouville derivatives in (3). We want to show that, by two-sided fractional derivatives, this method is also unconditionally stable and convergent.

### 2.1. Discretization of the STFDE

To start with, let  $m$  and  $n$  be two positive integers, and let  $h = (b - a)/m$  and  $\tau = T/n$  be the sizes of time step and spatial grid, respectively. Then the spatial and temporal partitions can be defined by

$$x_i = a + ih, \quad i = 0, 1, \dots, m; \quad t_j = j\Delta t, \quad j = 0, 1, \dots, n,$$

and for convenience, we shall denote henceforth

$$\begin{aligned} d_{+,i}^{(j)} &= d_+(x_i, t_j), \quad d_{-,i}^{(j)} = d_-(x_i, t_j), \quad e_{+,i}^{(j)} = e_+(x_i, t_j), \\ e_{-,i}^{(j)} &= e_-(x_i, t_j), \quad f_i^{(j)} = f(x_i, t_j), \quad \Delta_t u(x_i, t_j) = u(x_i, t_{j+1}) - u(x_i, t_j). \end{aligned}$$

Upon utilizing the forward difference formula, it is known that the time fractional derivative for  $0 < \alpha < 1$  can be approximated by [1],

$$\begin{aligned} \frac{\partial^\alpha u(x_i, t_{k+1})}{\partial t^\alpha} &= \frac{1}{\Gamma(1-\alpha)} \int_0^{t_{k+1}} \frac{\partial u(x_i, s)}{\partial s} \frac{ds}{(t_{k+1} - s)^\alpha} \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^k \left( \left( \frac{1}{\tau} \Delta_t u(x_i, t_j) + \mathcal{O}(\tau) \right) \int_{t_j}^{t_{j+1}} (t_{k+1} - s)^{-\alpha} ds \right) + \mathcal{O}(\tau^{2-\alpha}) \\ &= \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \sum_{j=0}^k a_j \Delta_t u(x_i, t_{k-j}) + \mathcal{O}(\tau^{2-\alpha}), \end{aligned} \quad (4)$$

where  $a_j = (j+1)^{1-\alpha} - j^{1-\alpha}$ ,  $j = 0, 1, \dots, n$ . Also, the Riemann-Liouville derivatives in (3) can be approximated by adopting the Grünwald estimates and the shifted Grünwald estimates (see [21, Remark 2.5]) for parameters  $\beta$  and  $\gamma$ , respectively, i.e.,

$$D_{a,x}^{(\beta)} u(x_i, t_{k+1}) = \frac{1}{h^\beta} \sum_{j=0}^i g_j^{(\beta)} u(x_{i-j}, t_{k+1}) + \mathcal{O}(h), \quad (5a)$$

$$D_{x,b}^{(\beta)} u(x_i, t_{k+1}) = \frac{1}{h^\beta} \sum_{j=0}^{m-i} g_j^{(\beta)} u(x_{i+j}, t_{k+1}) + \mathcal{O}(h), \quad (5b)$$

$$D_{a,x}^{(\gamma)} u(x_i, t_{k+1}) = \frac{1}{h^\gamma} \sum_{j=0}^{i+1} g_j^{(\gamma)} u(x_{i-j+1}, t_{k+1}) + \mathcal{O}(h), \quad (5c)$$

$$D_{x,b}^{(\gamma)} u(x_i, t_{k+1}) = \frac{1}{h^\gamma} \sum_{j=0}^{i+1} g_j^{(\gamma)} u(x_{i+j-1}, t_{k+1}) + \mathcal{O}(h), \quad (5d)$$

where

$$\begin{aligned} g_0^{(\beta)} &= 1, \quad g_j^{(\beta)} = \frac{(-1)^j}{j!} \beta(\beta-1) \cdots (\beta-j+1), \quad j = 1, 2, \dots, \\ g_0^{(\gamma)} &= 1, \quad g_j^{(\gamma)} = \frac{(-1)^j}{j!} \gamma(\gamma-1) \cdots (\gamma-j+1), \quad j = 1, 2, \dots \end{aligned}$$

Let

$$\omega_1 = \frac{\Gamma(2-\alpha)\tau^\alpha}{h^\beta}, \quad \omega_2 = \frac{\Gamma(2-\alpha)\tau^\alpha}{h^\gamma}, \quad \omega_3 = \Gamma(2-\alpha)\tau^\alpha,$$

and  $u_i^{(j)}$  represent the numerical approximation of  $u(x_i, t_j)$ . Using (4) and (5), we shall see that the solution of (1) can be approximated by the following *implicit difference method*:

$$\begin{aligned} u_i^{(k+1)} + \omega_1 \left( d_{+,i}^{(k+1)} \sum_{j=0}^i g_j^{(\beta)} u_{i-j}^{(k+1)} + d_{-,i}^{(k+1)} \sum_{j=0}^{m-i} g_j^{(\beta)} u_{i+j}^{(k+1)} \right) - \omega_2 \left( e_{+,i}^{(k+1)} \sum_{j=0}^{i+1} g_j^{(\gamma)} u_{i-j+1}^{(k+1)} \right. \\ \left. + e_{-,i}^{(k+1)} \sum_{j=0}^{m-i+1} g_j^{(\gamma)} u_{i+j-1}^{(k+1)} \right) = u_i^{(k)} - \sum_{j=1}^k a_j (u_i^{(k-j+1)} - u_i^{(k-j)}) + \omega_3 f_i^{(k+1)}, \end{aligned} \quad (6)$$

where  $i = 1, \dots, m-1$ ;  $k = 0, \dots, n-1$ , and the boundary and initial conditions can be discretized as follows:

$$u_i^{(0)} = \phi(x_i), \quad i = 0, \dots, m; \quad u_0^{(k)} = u_m^{(k)} = 0, \quad k = 1, \dots, n.$$

## 2.2. Analysis of the implicit difference method

To analyze the stability and convergence of the implicit difference method given above, we first let  $U_i^{(k)}$  be the approximation solution of  $u_i^{(k)}$  in (6), and let  $\xi_i^{(k)} = U_i^{(k)} - u_i^{(k)}$ ,  $i = 1, \dots, m-1$ ;  $k = 0, \dots, n-1$ , be the error satisfying the equation

$$\begin{aligned} \xi_i^{(k+1)} + \omega_1 \left( d_{+,i}^{(k+1)} \sum_{j=0}^i g_j^{(\beta)} \xi_{i-j}^{(k+1)} + d_{-,i}^{(k+1)} \sum_{j=0}^{m-i} g_j^{(\beta)} \xi_{i+j}^{(k+1)} \right) - \omega_2 \left( e_{+,i}^{(k+1)} \sum_{j=0}^{i+1} g_j^{(\gamma)} \xi_{i-j+1}^{(k+1)} \right. \\ \left. + e_{-,i}^{(k+1)} \sum_{j=0}^{m-i+1} g_j^{(\gamma)} \xi_{i+j-1}^{(k+1)} \right) = \xi_i^{(k)} - \sum_{j=1}^k a_j (\xi_i^{(k-j+1)} - \xi_i^{(k-j)}). \end{aligned} \quad (7)$$

Correspondingly, assume  $E^{(k+1)} = [\xi_1^{(k)}, \xi_2^{(k)}, \dots, \xi_{m-1}^{(k)}]^\top$ ,  $k = 0, \dots, n-1$ . It is obvious upon inspection that the method given by (6) is stable, once we can show that

$$\|E^{(k+1)}\|_\infty \leq \|E^{(0)}\|_\infty.$$

To this purpose, the following results given in [21, 22, 27] are required.

**Lemma 2.1.** *The coefficients  $a_j$ ,  $g_j^{(\beta)}$ ,  $g_j^{(\gamma)}$ , for  $j = 1, 2, \dots$ , satisfy*

1.  $1 = a_0 > a_1 > a_2 > \dots > a_j \rightarrow 0$ , as  $j \rightarrow \infty$ ,
2.  $g_0^{(\beta)} = 1$ ,  $g_j^{(\beta)} < 0$ , for  $j = 1, 2, \dots$ , and  $\sum_{j=0}^\infty g_j^{(\beta)} = 0$ ,
3.  $g_1^{(\gamma)} = -\gamma < 0$ ,  $g_j^{(\gamma)} > 0$ , for  $j \neq 1$ , and  $\sum_{j=0}^\infty g_j^{(\gamma)} = 0$ .
4.  $g_j^{(\beta)} = \mathcal{O}(j^{-(\beta+1)})$  and  $g_j^{(\gamma)} = \mathcal{O}(j^{-(\gamma+1)})$ .

We do want to note that Lemma 2.1 implies that

$$\sum_{j=0}^k g_j^{(\beta)} > 0 \text{ and } \sum_{j=0}^{k+1} g_j^{(\gamma)} < 0, \quad \text{for } k = 0, 1, \dots$$

This observation also gives rise to the certification of the stability of the method given by (6).

**Theorem 2.2.** *The implicit difference method (6) for time-space fractional diffusion equation is unconditionally stable, that is,*

$$\|E^{(k+1)}\|_\infty \leq \|E^{(0)}\|_\infty, \quad 0 \leq k \leq n-1. \quad (8)$$

**Proof:** First, without loss of generality, we may assume that the diffusion coefficient functions  $d_+(x, t) = d_+$ ,  $d_-(x, t) = d_-$ ,  $e_+(x, t) = e_+$  and  $e_-(x, t) = e_-$  are constants in our proof. Suppose that  $k = 0$ , and let  $\xi_\ell^{(1)} = \|E^{(1)}\|_\infty := \max_{1 \leq i \leq m-1} |\xi_i^{(1)}|$ . Then

$$\begin{aligned} |\xi_\ell^{(1)}| &\leq \left[ 1 + \omega_1 \left( d_{+, \ell}^{(k+1)} \sum_{j=0}^{\ell} g_j^{(\beta)} + d_{-, \ell}^{(k+1)} \sum_{j=0}^{m-\ell} g_j^{(\beta)} \right) - \omega_2 \left( e_{+, \ell}^{(k+1)} \sum_{j=0}^{\ell+1} g_j^{(\gamma)} + e_{-, \ell}^{(k+1)} \sum_{j=0}^{m-\ell+1} g_j^{(\gamma)} \right) \right] |\xi_\ell^{(1)}| \\ &\leq |\xi_\ell^{(1)}| + \omega_1 \left( d_{+, \ell}^{(1)} \sum_{j=0}^{\ell} g_j^{(\beta)} |\xi_{\ell-j}^{(1)}| + d_{-, \ell}^{(1)} \sum_{j=0}^{m-\ell} g_j^{(\beta)} |\xi_{\ell+j}^{(1)}| \right) - \omega_2 \left( e_{+, \ell}^{(1)} \sum_{j=0}^{\ell+1} g_j^{(\gamma)} |\xi_{\ell-j+1}^{(1)}| + e_{-, \ell}^{(1)} \sum_{j=0}^{m-\ell+1} g_j^{(\gamma)} |\xi_{\ell+j-1}^{(1)}| \right) \\ &\leq \left| \xi_\ell^{(1)} + \omega_1 \left( d_{+, \ell}^{(1)} \sum_{j=0}^{\ell} g_j^{(\beta)} \xi_{\ell-j}^{(1)} + d_{-, \ell}^{(1)} \sum_{j=0}^{m-\ell} g_j^{(\beta)} \xi_{\ell+j}^{(1)} \right) - \omega_2 \left( e_{+, \ell}^{(1)} \sum_{j=0}^{\ell+1} g_j^{(\gamma)} \xi_{\ell-j+1}^{(1)} + e_{-, \ell}^{(1)} \sum_{j=0}^{m-\ell+1} g_j^{(\gamma)} \xi_{\ell+j-1}^{(1)} \right) \right| \\ &= |\xi_\ell^{(0)}| \leq \|E^{(0)}\|_\infty. \end{aligned}$$

Here, the second and third inequalities are true due to the fact given in Lemma 2.1 and the triangle inequality on absolute value. Now suppose that for some integer  $k \geq 0$ , the result is established, i.e.,

$$\|E^{(j)}\|_\infty \leq \|E^{(0)}\|_\infty, \quad \text{for } j \leq k.$$

As we did earlier for  $k = 0$ , let  $\xi_\ell^{(k+1)} = \max_{1 \leq i \leq m-1} |\xi_i^{(k+1)}|$ . By Lemma 2.1, it can be seen that

$$\begin{aligned} |\xi_\ell^{(k+1)}| &\leq \left| \xi_\ell^{(k+1)} + \omega_1 \left( d_{+, \ell}^{(k+1)} \sum_{j=0}^{\ell} g_j^{(\beta)} \xi_{\ell-j}^{(k+1)} + d_{-, \ell}^{(k+1)} \sum_{j=0}^{m-\ell} g_j^{(\beta)} \xi_{\ell+j}^{(k+1)} \right) \right. \\ &\quad \left. - \omega_2 \left( e_{+, \ell}^{(k+1)} \sum_{j=0}^{\ell+1} g_j^{(\gamma)} \xi_{\ell-j+1}^{(k+1)} + e_{-, \ell}^{(k+1)} \sum_{j=0}^{m-\ell+1} g_j^{(\gamma)} \xi_{\ell+j-1}^{(k+1)} \right) \right| \\ &= \left| \xi_\ell^k - \sum_{j=1}^k a_j (\xi_\ell^{k-j+1} - \xi_\ell^{k-j}) \right| = \left| \sum_{j=1}^k (a_{j-1} - a_j) \xi_\ell^{(k-j+1)} + a_k \xi_\ell^{(0)} \right| \\ &\leq \|E^{(0)}\|_\infty. \end{aligned}$$

Truly, the preceding result, which follows from the assumption that the coefficient functions are constant, does not provide complete results. In fact, it can be seen that the above proof requires only the properties of non-negatives of the coefficient functions. Thus, the result for non-constant ones can be proved similarly.

□

Our next theorem is to analyze the convergence of the implicit method given in (6). To this end, recall that  $u(x_i, t_j)$ ,  $i = 1, \dots, n-1$ ;  $j = 0, \dots, n-1$ , denotes the exact solution of (1) at mesh point  $(x_i, t_j)$  and  $u_i^{(j)}$ ,  $i = 1, \dots, n-1$ ;  $j = 0, \dots, n-1$ , represents the solution of (6). Let us assume that  $\psi_i^{(k)} = u(x_i, t_k) - u_i^{(k)}$  and  $\Psi^{(k)} = (\psi_1^{(k)}, \psi_2^{(k)}, \dots, \psi_{m-1}^{(k)})^\top$ . Note that, by construction,  $\Psi^{(0)} = \mathbf{0}$ , since  $u_i^{(0)} = \psi(x_i) = u(x_i, 0)$ ,  $i = 1, \dots, m-1$ .

Using this notation, we consider

$$\begin{cases} \psi_i^{(1)} + \omega_1 \left( d_{+,i}^{(1)} \sum_{j=0}^i g_j^{(\beta)} \psi_{i-j}^{(1)} + d_{-,i}^{(1)} \sum_{j=0}^{m-i} g_j^{(\beta)} \psi_{i+j}^{(1)} \right) - \omega_2 \left( e_{+,i}^{(1)} \sum_{j=0}^{i+1} g_j^{(\gamma)} \psi_{i-j+1}^{(1)} \right. \\ \left. + e_{-,i}^{(1)} \sum_{j=0}^{m-i+1} g_j^{(\gamma)} \psi_{i+j-1}^{(1)} \right) = R_i^{(1)}, \\ \psi_i^{(k+1)} + \omega_1 \left( d_{+,i}^{(k+1)} \sum_{j=0}^i g_j^{(\beta)} \psi_{i-j}^{(k+1)} + d_{-,i}^{(k+1)} \sum_{j=0}^{m-i} g_j^{(\beta)} \psi_{i+j}^{(k+1)} \right) - \omega_2 \left( e_{+,i}^{(k+1)} \sum_{j=0}^{i+1} g_j^{(\gamma)} \right. \\ \left. \psi_{i-j+1}^{(k+1)} + e_{-,i}^{(k+1)} \sum_{j=0}^{m-i+1} g_j^{(\gamma)} \psi_{i+j-1}^{(k+1)} \right) = \psi_i^{(k)} - \sum_{j=1}^k a_j (\psi_i^{(k-j+1)} - \psi_i^{(k-j)}) + R_i^{(k+1)}, \\ 1 \leq i \leq m-1, 1 \leq k \leq n-1. \end{cases} \quad (9)$$

In this way, we can observe from (4) and (5) that

$$R_i^{(k+1)} = \mathcal{O}((\tau^2 + \tau^\alpha h)), \quad 1 \leq i \leq m-1; 0 \leq k \leq n-1. \quad (10)$$

Thus, a way to do the convergence analysis is sufficed to come up with an upper bound of  $\|\Psi^{(k+1)}\|_\infty$ ,  $k = 0, 1, \dots, n-1$ , as follows.

**Theorem 2.3.**

$$\|\Psi^{(k+1)}\|_\infty \leq C a_k^{-1} (\tau^2 + \tau^\alpha h), \quad k = 0, \dots, n-1, \quad (11)$$

for some constant  $C$ .

**Proof:** Corresponding to (10), we shall assume for convenience that there is a positive constant  $C$  such that

$$|R_i^{(k+1)}| \leq C(\tau^2 + \tau^\alpha h), \quad 1 \leq i \leq m-1; 0 \leq k \leq n-1.$$

Then, the poof is by mathematical induction on  $k$ . Let  $|\psi_\ell^1| = \|\Psi^1\|_\infty := \max_{1 \leq i \leq m-1} |\psi_i^1|$ . Observe

from (9) that if  $k = 0$ , then we have

$$\begin{aligned}
|\psi_\ell^{(1)}| &\leq \left[ 1 + \omega_1 \left( d_{+,\ell}^{(k+1)} \sum_{j=0}^{\ell} g_j^{(\beta)} + d_{-,\ell}^{(k+1)} \sum_{j=0}^{m-\ell} g_j^{(\beta)} \right) - \omega_2 \left( e_{+,\ell}^{(k+1)} \sum_{j=0}^{\ell+1} g_j^{(\gamma)} + e_{-,\ell}^{(k+1)} \sum_{j=0}^{m-\ell+1} g_j^{(\gamma)} \right) \right] |\psi_\ell^{(1)}| \\
&\leq |\psi_\ell^{(1)}| + \omega_1 \left( d_{+,\ell}^{(1)} \sum_{j=0}^{\ell} g_j^{(\beta)} |\psi_{\ell-j}^{(1)}| + d_{-,\ell}^{(1)} \sum_{j=0}^{m-\ell} g_j^{(\beta)} |\psi_{\ell+j}^{(1)}| \right) - \omega_2 \left( e_{+,\ell}^{(1)} \sum_{j=0}^{\ell+1} g_j^{(\gamma)} |\psi_{\ell-j+1}^{(1)}| + e_{-,\ell}^{(1)} \sum_{j=0}^{m-\ell+1} g_j^{(\gamma)} |\psi_{\ell+j-1}^{(1)}| \right) \\
&\leq \left| \psi_\ell^{(1)} + \omega_1 \left( d_{+,\ell}^{(1)} \sum_{j=0}^{\ell} g_j^{(\beta)} \psi_{\ell-j}^{(1)} + d_{-,\ell}^{(1)} \sum_{j=0}^{m-\ell} g_j^{(\beta)} \psi_{\ell+j}^{(1)} \right) - \omega_2 \left( e_{+,\ell}^{(1)} \sum_{j=0}^{\ell+1} g_j^{(\gamma)} \psi_{\ell-j+1}^{(1)} + e_{-,\ell}^{(1)} \sum_{j=0}^{m-\ell+1} g_j^{(\gamma)} \psi_{\ell+j-1}^{(1)} \right) \right| \\
&= |R_\ell^{(1)}| \leq C a_0^{-1} (\tau^2 + \tau^\alpha h),
\end{aligned}$$

namely,

$$\|\Psi^1\|_\infty \leq C a_0^{-1} (\tau^2 + \tau^\alpha h),$$

Suppose that the result is valid for some integer  $k \geq 0$ , i.e.,

$$\|\Psi^j\|_\infty \leq C a_{k-1}^{-1} (\tau^2 + \tau^\alpha h), \quad j = 1, \dots, k-1. \quad (12)$$

Let  $|\psi_\ell^{k+1}| = \|\Psi^{k+1}\|_\infty := \max_{1 \leq i \leq m-1} |\psi_i^{k+1}|$ . It follows that

$$\begin{aligned}
|\psi_\ell^{k+1}| &\leq \left| \psi_\ell^{(k+1)} + \omega_1 \left( d_{+,\ell}^{(k+1)} \sum_{j=0}^{\ell} g_j^{(\beta)} \psi_{\ell-j}^{(k+1)} + d_{-,\ell}^{(k+1)} \sum_{j=0}^{m-\ell} g_j^{(\beta)} \psi_{\ell+j}^{(k+1)} \right) \right. \\
&\quad \left. - \omega_2 \left( e_{+,\ell}^{(k+1)} \sum_{j=0}^{\ell+1} g_j^{(\gamma)} \psi_{\ell-j+1}^{(k+1)} + e_{-,\ell}^{(k+1)} \sum_{j=0}^{m-\ell+1} g_j^{(\gamma)} \psi_{\ell+j-1}^{(k+1)} \right) \right| \\
&= \left| \psi_\ell^k - \sum_{j=1}^k a_j (\psi_\ell^{k-j+1} - \psi_\ell^{k-j}) \right| = \left| \sum_{j=1}^k (a_{j-1} - a_j) \psi_\ell^{(k-j+1)} + a_k \psi_\ell^{(0)} + R_\ell^{(k+1)} \right| \\
&\leq \sum_{j=1}^k (a_{j-1} - a_j) |\psi_\ell^{(k-j+1)}| + |R_\ell^{(k+1)}| \\
&\leq C \left( a_k + \sum_{j=1}^k (a_{j-1} - a_j) \right) a_k^{-1} (\tau^2 + \tau^\alpha h) \leq C a_k^{-1} (\tau^2 + \tau^\alpha h),
\end{aligned}$$

since  $a_{j-1} - a_j > 0$ ,  $j = 1, \dots, k$ , and  $\psi_\ell^{(0)} = 0$ . □

It has been shown in [1] that

$$\lim_{k \rightarrow \infty} \frac{a_k^{-1}}{k^\alpha} = \frac{1}{1 - \alpha}. \quad (13)$$

By (11) and (13), we immediately have the following result, which demonstrates the convergence of our implicit method.



**Corollary 2.4.** Let  $u_i^{(k)}$ ,  $i = 1, \dots, m-1$ ;  $k = 1, \dots, n$  be the numerical solution computed by the implicit difference method (6). Then, there exists a constant  $C$  such that

$$|u(x_i, t_k) - u_i^{(k)}| \leq C(\tau^{2-\alpha} + h), \quad i = 1, \dots, m-1; k = 1, \dots, n. \quad (14)$$

We remark that the above approach used to analyze the stability and convergence is simply a follow-up used by Liu *et al.* in [1]. Our focus in this work is to apply the efficient CGNR method and GMRES method to solve the linear system arised from (6) in terms of suitably constructed preconditioners.

### 3. Preconditioned iterative methods

Before moving into the investigation of preconditioning techniques, the matrix representation of (6) should be elaborated first. To facilitate our discussion, we use  $I_{m-1}$  to denote the identity matrix of order  $m-1$ . For  $1 \leq j \leq n-1$ , let

$$\begin{aligned} \mathbf{u}^{(j)} &= [u_1^{(j)}, u_2^{(j)}, \dots, u_{m-1}^{(j)}]^\top, \quad \mathbf{f}^{(j)} = [f_1^{(j)}, f_2^{(j)}, \dots, f_{m-1}^{(j)}]^\top, \\ D_+^{(j)} &= \text{diag}(d_{+,1}^{(j)}, \dots, d_{+,m-1}^{(j)}), \quad D_-^{(j)} = \text{diag}(d_{-,1}^{(j)}, \dots, d_{-,m-1}^{(j)}), \\ E_+^{(j)} &= \text{diag}(e_{+,1}^{(j)}, \dots, e_{+,m-1}^{(j)}), \quad E_-^{(j)} = \text{diag}(e_{-,1}^{(j)}, \dots, e_{-,m-1}^{(j)}), \end{aligned}$$

and  $\mathbf{u}^{(0)} = (\phi_1^{(0)}, \phi_2^{(0)}, \dots, \phi_{m-1}^{(0)})^\top$ . Let  $G_\beta$  and  $G_\gamma$  be two Toeplitz matrices defined by

$$G_\beta = \begin{bmatrix} g_0^{(\beta)} & 0 & \cdots & \cdots & 0 \\ g_1^{(\beta)} & g_0^{(\beta)} & 0 & \cdots & 0 \\ \vdots & g_1^{(\beta)} & g_0^{(\beta)} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ g_{m-2}^{(\beta)} & \ddots & \ddots & \ddots & g_0^{(\beta)} \end{bmatrix}, \quad G_\gamma = \begin{bmatrix} g_1^{(\gamma)} & g_0^{(\gamma)} & 0 & \cdots & 0 & 0 \\ g_2^{(\gamma)} & g_1^{(\gamma)} & g_0^{(\gamma)} & 0 & \cdots & 0 \\ \vdots & g_2^{(\gamma)} & g_1^{(\gamma)} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ g_{m-2}^{(\gamma)} & \ddots & \ddots & \ddots & g_1^{(\gamma)} & g_0^{(\gamma)} \\ g_{m-1}^{(\gamma)} & g_{m-2}^{(\gamma)} & \cdots & \cdots & g_2^{(\gamma)} & g_1^{(\gamma)} \end{bmatrix}.$$

Upon substitution, we see that (6) is equivalent to a matrix equation of the form

$$(I_{m-1} + A^{(k+1)})\mathbf{u}^{(k+1)} = \mathbf{b}^{(k+1)}, \quad (15)$$

where

$$\mathbf{b}^{(k+1)} = \sum_{j=1}^k (a_{k-j} - a_{k-j+1})\mathbf{u}^{(j)} + a_k \mathbf{u}^{(0)} + \omega_3 \mathbf{f}^{k+1}$$

and

$$A^{(k+1)} = \omega_1 (D_+^{(k+1)} G_\beta + D_-^{(k+1)} G_\beta^\top) - \omega_2 (E_+^{(k+1)} G_\gamma + E_-^{(k+1)} G_\gamma^\top). \quad (16)$$

Now we can define the corresponding matrix equation of (6). An intuitive question to ask is whether the matrix equation is uniquely solvable. Before answering this, we make an interesting observation of the following result.

**Theorem 3.1.** *The matrix  $I_{m-1} + A^{(k+1)}$  in (15) is a nonsingular, strictly diagonally dominant  $M$ -matrix.*

**Proof:** Let  $a_{ij}^{(k+1)}$  be the  $(i, j)$  entry of the matrix  $A^{(k+1)}$  in (15). Note that we have from (15),

$$\begin{aligned}
& a_{ii}^{(k+1)} - \sum_{j=1, j \neq i}^{m-1} |a_{ij}^{(k+1)}| \\
&= \omega_1 \left( d_{+,i}^{(k+1)} + d_{-,i}^{(k+1)} \right) g_0^{(\beta)} - \omega_1 \left( d_{+,i}^{(k+1)} \sum_{j=1}^{i-1} g_j^{(\beta)} + d_{-,i}^{(k+1)} \sum_{j=1}^{m-i-1} g_j^{(\beta)} \right) \\
& \quad - \omega_2 \left( e_{+,i}^{(k+1)} + e_{-,i}^{(k+1)} \right) g_1^{(\gamma)} - \omega_2 \left( e_{+,i}^{(k+1)} \sum_{j=0, j \neq 1}^i g_j^{(\gamma)} + e_{-,i}^{(k+1)} \sum_{j=0, j \neq 1}^{m-i} g_j^{(\gamma)} \right) \quad (17) \\
& \geq \omega_1 \left( d_{+,i}^{(k+1)} + d_{-,i}^{(k+1)} \right) g_0^{(\beta)} - \omega_1 \left( d_{+,i}^{(k+1)} + d_{-,i}^{(k+1)} \right) \sum_{j=1}^{\infty} g_j^{(\beta)} \\
& \quad - \omega_2 \left( e_{+,i}^{(k+1)} + e_{-,i}^{(k+1)} \right) g_1^{(\gamma)} - \omega_2 \left( e_{+,i}^{(k+1)} + e_{-,i}^{(k+1)} \right) \sum_{j=0, j \neq 1}^{\infty} g_j^{(\gamma)} = 0.
\end{aligned}$$

At first glance, this implies that the coefficient matrix  $I_{m-1} + A^{(k+1)}$  is strictly diagonally dominant and  $(I_{m-1} + A^{(k+1)})\mathbf{1} > 0$ , where  $\mathbf{1}$  is a vector of length  $n - 1$  with all entries equal to one. We observe further that  $a_{i,j} \leq 0$ , for all  $i \neq j$ , that is, the matrix  $I_{m-1} + A^{(k+1)}$  is a  $Z$ -matrix. This completes the proof.  $\square$

With the aid of Lemma 3.1, we can point out quickly that the solution of (15) is unique. More significantly, since (15) is a matrix representation of (6), we then come up with the following result.

**Corollary 3.2.** *The difference method (6) is uniquely solvable.*

By now, we have completed the proof of the unique solvability of the implicit difference scheme given in (6). We are now ready to apply the popular and effective iterative methods, the CGNR and GMRES methods, to solve (15). In section 4, we will see that while solving large-scale equations, the systems would become nearly singular and ill-conditioned. For such problems, we apply the preconditioner technique to accelerate the iterative process.

To this purpose, we start by decomposing matrices  $G_\beta$  and  $G_\gamma$  as

$$G_\beta = G_{\beta,\ell} + (G_\beta - G_{\beta,\ell}),$$

$$G_\gamma = G_{\gamma,\ell} + (G_\gamma - G_{\gamma,\ell}),$$

where

$$\begin{aligned}
G_{\beta,\ell} &= \begin{bmatrix} g_0^{(\beta)} & & & & \\ \vdots & g_0^{(\beta)} & & & \\ g_{\ell-1}^{(\beta)} & & \ddots & & \\ & \ddots & & \ddots & \\ & & g_{\ell-1}^{(\beta)} & \cdots & g_0^{(\alpha)} \end{bmatrix} + \begin{bmatrix} 0 & & & & \\ & \ddots & & & \\ & & 0 & & \\ & & & g_{\ell}^{(\beta)} & \\ & & & & \ddots \\ & & & & & \sum_{j=\ell}^{m-2} g_j^{(\beta)} \end{bmatrix}, \\
G_{\gamma,\ell} &= \begin{bmatrix} g_1^{(\gamma)} & g_0^{(\gamma)} & & & \\ \vdots & g_1^{(\gamma)} & g_0^{(\gamma)} & & \\ g_{\ell}^{(\gamma)} & & \ddots & \ddots & \\ & \ddots & & \ddots & g_0^{(\alpha)} \\ & & g_{\ell}^{(\gamma)} & \cdots & g_1^{(\gamma)} \end{bmatrix} + \begin{bmatrix} 0 & & & & \\ & \ddots & & & \\ & & 0 & & \\ & & & g_{\ell+1}^{(\gamma)} & \\ & & & & \ddots \\ & & & & & \sum_{j=\ell+1}^{m-1} g_j^{(\gamma)} \end{bmatrix}.
\end{aligned}$$

Namely, the matrix  $A^{(k+1)}$  can be decomposed as

$$A^{(k+1)} = A_{\ell}^{(k+1)} + B_{\ell}^{(k+1)},$$

where

$$\begin{aligned}
A_{\ell}^{(k+1)} &= \omega_1(D_+^{k+1}G_{\beta,\ell} + D_-^{k+1}G_{\beta,\ell}^{\top}) - \omega_2(E_+^{k+1}G_{\gamma,\ell} + E_-^{k+1}G_{\gamma,\ell}^{\top}), \\
B_{\ell}^{(k+1)} &= A^{(k+1)} - A_{\ell}^{(k+1)}.
\end{aligned}$$

Note that from Lemma 2.1, it is easy to show that the Toeplitz matrices  $G_{\beta}$  and  $-G_{\gamma}$  are  $M$ -matrices and strictly diagonally dominant. This implies that the matrices  $G_{\beta,\ell}$  and  $G_{\gamma,\ell}$  are thus strictly diagonally dominant  $M$ -matrices, since the matrices  $G_{\beta,\ell}$  and  $G_{\gamma,\ell}$  have the same row sums as  $G_{\beta}$  and  $G_{\gamma}$ , respectively. In this way, the following fact can be realized directly.

**Theorem 3.3.** *The matrix  $I_{m-1} + A_{\ell}^{(k+1)}$  is a nonsingular, strictly diagonally dominant  $M$ -matrix for all  $\ell$ .*

In addition, Lemma 2.1 implies that

$$\begin{aligned}
&\frac{\|(I_{m-1} + A^{(k+1)}) - (I_{m-1} + A_{\ell}^{(k+1)})\|_{\infty}}{\|I_{m-1} - A^{(k+1)}\|_{\infty}} \\
&\leq \frac{\frac{1}{h^{\beta}}\|(D_+^{k+1}(G_{\beta} - G_{\beta,\ell}) + D_-^{k+1}(G_{\beta} - G_{\beta,\ell})^{\top}) - (E_+^{k+1}(G_{\gamma} - G_{\gamma,\ell}) + E_-^{k+1}(G_{\gamma} - G_{\gamma,\ell})^{\top})\|_{\infty}}{\frac{1}{h^{\beta}}\|(D_+^{(k+1)}G_{\beta} + D_-^{(k+1)}G_{\beta}^{\top}) - (E_+^{(k+1)}G_{\gamma} + E_-^{(k+1)}G_{\gamma}^{\top})\|_{\infty}} = O(k^{-\beta}),
\end{aligned}$$

since  $\|G_\beta - G_{\beta,\ell}\|_\infty = \mathcal{O}(k^{-\beta})$ ,  $\|G_\gamma - G_{\gamma,\ell}\|_\infty = \mathcal{O}(k^{-\gamma})$ , and  $h = (b - a)/m$  [33]. Namely, the relative difference between  $I_{m-1} + A^{(k+1)}$  and  $I_{m-1} + A_\ell^{(k+1)}$  can become very small while  $k$  becomes large enough. Observe further that the banded matrix  $I_{m-1} + A_\ell^{(k+1)}$  is a sparse matrix consisting of  $2\ell - 1$  nonzero diagonal entries. With this in hand, an efficient preconditioner for the linear system (15) is attainable by simply choosing  $I_{m-1} + A_\ell^{(k+1)}$ . We assume here that the reader is familiar with the fundamental terminology and iterative approaches of the preconditioned GMRES and CGNR methods. For a comprehensive understanding of such iterative techniques, the reader is referred to the monograph [34] written by Saad.

### 3.1. Preconditioned GMRES method

The GMRES method, proposed in 1986 in [35], is one of the most popular and effective methods for solving nonsymmetric linear systems. However, for large sparse systems, one might try to apply preconditioning techniques to reduce the condition number, and hence improve the convergence rate. Let  $P_\ell^{(k+1)} := I_{m-1} + A_\ell^{(k+1)}$ . Our purpose here is to replace the linear system (15) by the preconditioned linear system

$$(P_\ell^{(k+1)})^{-1}(I_{m-1} + A^{(k+1)})\mathbf{u}^{(k+1)} = (P_\ell^{(k+1)})^{-1}\mathbf{b}^{(k+1)} \quad (18)$$

with the same solution. We then solve (18) in terms of the left-preconditioned GMRES method proposed in [33]. To make this work more self-contained, we quote this method as follows:

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#### Preconditioned GMRES( $\rho$ ) method

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At each time step  $t^{(k+1)}$ , we choose  $\mathbf{u}_0$  as initial guess for  $\mathbf{u}^{(k+1)}$

Set  $\mu := 0$ , and compute the LU factorization:  $P_\ell^{(k+1)} = LU$

Compute  $\mathbf{r} := \mathbf{b}^{(k+1)} - (I_{m-1} + A^{(k+1)})\mathbf{u}^{(k+1)}$ , and assign  $\mathbf{r}_t := \mathbf{r}$

While  $\mu \leq IterMax$  and  $\|\mathbf{r}_t\|_2 / \|\mathbf{b}^{(k+1)}\|_2 > \epsilon$  do

$\mu := \mu + 1$

Compute  $\mathbf{r}_w := U^{-1}L^{-1}\mathbf{r}$ ,  $\beta := \|\mathbf{r}_w\|$ ,  $\mathbf{v}_1 := \mathbf{r}_w/\beta$

Assign  $j := 0$  and  $V_1 := \mathbf{v}_1$

While  $j \leq \rho$  and  $\|\mathbf{r}_t\|_2 / \|\mathbf{b}^{(k+1)}\|_2 > \epsilon$  do

$j := j + 1$

Compute  $\mathbf{w} := U^{-1}L^{-1}(I_{m-1} + A^{(k+1)})\mathbf{v}_j$

For  $i = 1, \dots, j$  do

$h_{i,j} = \mathbf{v}_i^T * \mathbf{w}$

$\mathbf{w} := \mathbf{w} - h_{i,j}\mathbf{v}_i$

Enddo

Compute  $h_{j+1,j} = \|\mathbf{w}\|_2$  and  $\mathbf{v}_{j+1} := \mathbf{w}/h_{j+1,j}$

---

```

Assign  $V_{j+1} := [V_j, \mathbf{v}_{j+1}]$  and  $H_j := [h_{\gamma, \delta}]_{1 \leq \gamma \leq j+1, 1 \leq \delta \leq j}$ 
Compute  $\mathbf{y}_j := \operatorname{argmin}_{\mathbf{y}} \|\beta \mathbf{e}_1 - H_j \mathbf{y}\|_2$ 
Compute the residual  $\mathbf{r}_t := \mathbf{r} - LU V_{j+1} H_j \mathbf{y}_j$ 
Enddo
 $\mathbf{r} := \mathbf{r}_t$ 
 $\mathbf{u}^{(k+1)} := \mathbf{u}^{(k+1)} + V_j \mathbf{y}_j$ 
Enddo

```

---

Here,  $IterMax$  denotes the maximal number of iteration,  $\epsilon$  denotes the given relative accuracy of the residual,  $\rho$  denotes that the GMRES method is restarted after  $\rho$  iterations, and the symbols  $\mathbf{r}_t$  and  $\mathbf{r}_w$  represent the current residual of the original linear system (15) and that of the preconditioned linear system (18), accordingly. Associated with this preconditioned method, two major portions of the computational work are:

- the computation of  $\mathbf{w} = U^{-1} L^{-1} (I_{m-1} + A^{(k+1)}) \mathbf{v}_j$  and
- the computation of  $\mathbf{r}_t = \mathbf{r} - LU V_{j+1} H_j \mathbf{y}_j$ .

We observe from (16) that

$$A^{(k+1)} \mathbf{v} = \omega_1 (D_+^{(k+1)} G_\beta \mathbf{v} + D_-^{(k+1)} G_\beta^\top \mathbf{v}) - \omega_2 (E_+^{(k+1)} G_\gamma \mathbf{v} + E_-^{(k+1)} G_\gamma^\top \mathbf{v}),$$

where  $G_\gamma$  and  $G_\beta$  are two  $(m-1)$ -by- $(m-1)$  Toeplitz matrices and can be stored only with  $m-1$  and  $m$  entries, respectively. This implies that the major work for computing  $A^{(k+1)} \mathbf{v}$  includes four Toeplitz matrix-vector multiplications,  $G_\beta \mathbf{v}$ ,  $G_\beta^\top \mathbf{v}$ ,  $G_\gamma \mathbf{v}$  and  $G_\gamma^\top \mathbf{v}$ , which can be obtained by using the fast Fourier transform (FFT) with only  $\mathcal{O}((m-1) \log(m-1))$  operations [28, 30, 36]. What might be important to note is that based on the specific structure of the matrix  $G_s$ , where  $s = \beta$  or  $\gamma$ , the calculations of  $G_s \mathbf{v}$  and  $G_s^\top \mathbf{v}$  can be done simultaneously, by computing  $G_\beta(\mathbf{v} + \sqrt{-1} \hat{\mathbf{v}})$ , where  $\hat{\mathbf{v}} = (v_{m-1}, v_{m-2}, \dots, v_1)^\top$ .

Since the matrix  $P_\ell^{(k+1)}$  is banded and strongly diagonally dominant,  $P_\ell^{(k+1)}$  admits a banded  $LU$  factorization [37, Proposition 2.3], i.e.,

$$P_\ell^{(k+1)} = LU, \tag{19}$$

where  $L$  and  $U$  are banded with bandwidth  $\ell$  and can be obtained in about  $\mathcal{O}((m-1)\ell^2)$  operations when  $\ell$  is small compared to  $(m-1)$ . This implies that given a vector  $\mathbf{x}$  of an appropriate size, the matrix-vector multiplications  $L\mathbf{x}$ ,  $U\mathbf{x}$ ,  $L^{-1}\mathbf{x}$ , and  $U^{-1}\mathbf{x}$  require only  $\mathcal{O}((m-1)\ell)$  operations. Thus, the computation of the vector  $\mathbf{w}$  requires  $\mathcal{O}((m-1) \log(m-1))$  operations, and the computation of the vector  $\mathbf{r}_t$  requires  $\mathcal{O}((m-1)(j+\ell))$  operations since  $V_{j+1}$  and  $H_j$  are matrices of sizes  $(m-1)$ -by- $(j+1)$  and  $(j+1)$ -by- $j$ .

### 3.2. Preconditioned CGNR method

For solving the nonsymmetric linear system (15), one might consider the application of the conjugate gradient (CG) method to the normal equation

$$(I_{m-1} + A^{(k+1)})^\top (I_{m-1} + A^{(k+1)}) \mathbf{u}^{(k+1)} = (I_{m-1} + A^{(k+1)})^\top \mathbf{b}^{(k+1)}. \quad (20)$$

This approach is known as CGNR. One disadvantage of applying the CG method directly to the equation (20) is that the condition number of  $(I_{m-1} + A^{(k+1)})^\top (I_{m-1} + A^{(k+1)})$  is the square of that of  $I_{m-1} + A^{(k+1)}$ . Thus, the convergence process of the CGNR method would be very slow. To accelerate the entire process, we choose  $(P_\ell^{(k+1)})^\top P_\ell^{(k+1)}$  as the preconditioner for the normal equation (20).

Note that the main computational works in the preconditioned CGNR method include two parts [34]. One is the matrix-vector multiplication  $(I_{m-1} + A^{(k+1)})^\top (I_{m-1} + A^{(k+1)}) \mathbf{v}$  for some vector  $\mathbf{v}$ . The other is the calculation of the solution of the linear system  $(P_\ell^{(k+1)})^\top P_\ell^{(k+1)} \mathbf{w} = \mathbf{z}$  for some vectors  $\mathbf{w}$  and  $\mathbf{z}$ . Of course, like the preconditioned GMRES method, the calculation of the matrix-vector multiplication  $(I_{m-1} + A^{(k+1)})^\top (I_{m-1} + A^{(k+1)}) \mathbf{v}$  can be done efficiently by applying the fast algorithm, FFT, to the Toeplitz-like structure of the resulting matrix  $A^{(k+1)}$  with  $\mathcal{O}((m-1)\log(m-1))$  operations. Similarly, from (19), we know that the solution of  $(P_\ell^{(k+1)})^\top P_\ell^{(k+1)} \mathbf{w} = \mathbf{z}$  can be obtained with only  $\mathcal{O}((m-1)\ell)$  operations.

## 4. Numerical experiments

In this section, we present an example to demonstrate the performance of preconditioned iterative methods versus unconditioned iterative methods. For all methods, the initial values are chosen to be

$$\mathbf{v}_0 = \begin{cases} \mathbf{u}^{(0)} := [\phi(x_1), \dots, \phi(x_{m-1})]^\top, & k = 1, \\ 2\mathbf{u}^{(k)} - \mathbf{u}^{(k-1)}, & k > 1. \end{cases}$$

as suggested in [27] and the stopping criterion is

$$\frac{\|\mathbf{r}_j\|_2}{\|\mathbf{b}^{(k+1)}\|_2} < 10^{-7},$$

where  $\mathbf{r}_j$  is the residual vector after  $j$ th iteration.

**Example 4.1.** Consider the equation (1) with  $\alpha = 0.8$ ,  $\beta = 0.6$ , and  $\gamma = 1.8$ . The left-sided and right-sided diffusion coefficients are given by

$$\begin{aligned} d_+(x, t) &= 6(1+t)x^{0.6}, & d_-(x, t) &= 6(1+t)(1-x)^{0.6}, \\ e_+(x, t) &= 6(1+t)x^{1.8}, & e_-(x, t) &= 6(1+t)(1-x)^{1.8}. \end{aligned}$$

with the spatial interval  $\Omega = (0, 1) \times (0, 1)$  and the time interval  $[0, T] = [0, 1]$ . The source term and the initial condition are given by

$$f(x, t) = e^t \left[ 6(1+t) \left( \left( \frac{\Gamma(4)}{\Gamma(3.4)} - \frac{\Gamma(4)}{\Gamma(2.2)} \right) (x^3 + (1-x)^3) - \left( \frac{3\Gamma(5)}{\Gamma(4.4)} - \frac{3\Gamma(5)}{\Gamma(3.2)} \right) (x^4 + (1-x)^4) \right. \right. \\ \left. \left. + \left( \frac{3\Gamma(6)}{\Gamma(5.4)} - \frac{3\Gamma(6)}{\Gamma(4.2)} \right) (x^5 + (1-x)^5) - \left( \frac{\Gamma(7)}{\Gamma(6.4)} - \frac{\Gamma(7)}{\Gamma(5.2)} \right) (x^6 + (1-x)^6) \right) + x^3(1-x)^3 \right]$$

and

$$u(x, 0) = x^3(1-x)^3.$$

It can be shown by a direct computation that the solution to the fractional diffusion equation is

$$u(x, t) = e^t x^3(1-x)^3.$$

Table 1: The average number of iterations for Example 4.1

$m = n$	GMRES(20)	PGMRES(20)	CGNR	PCGMR	error
16	8.000	3.063	12.438	3,125	$4.6312 \times 10^{-4}$
32	16.000	3.938	32.594	4.063	$2.4162 \times 10^{-4}$
64	84.969	4.063	100.547	4.813	$1.3320 \times 10^{-4}$
128	231.781	5.055	318.852	4.797	$7.5522 \times 10^{-5}$
256	486.859	6.082	1060.191	5.148	$4.5765 \times 10^{-5}$

Table 2: The required CPU times for Example 4.1

$m = n$	GMRES(20)	PGMRES(20)	CGNR	PCGMR
16	0.0046	0.0310	0.0620	0.0320
32	0.1400	0.0470	0.2810	0.0780
64	1.4510	0.1560	1.7000	0.1870
128	10.9200	0.5930	18.2210	0.7330
256	55.5830	3.7120	162.7550	4.1340

The numerical results were obtained by using MATLAB R2010a on a Lenovo Laptop Intel(R) Core(TM)2 Duo of 2.20 GHz CPU and 2GB RAM. We set the bandwidth  $\ell$  of the preconditioner  $P_\ell^{(k+1)}$  equal to 8 and use “ $m$ ” and “ $n$ ” to represent the numbers of the spatial partition and

Table 3: Condition numbers for relevant matrices for Example 4.1.

$m = n$	16	32	64	128	256
$k(\hat{A})$	48.86	162.84	491.07	1.34e+3	3.34e+3
$k((P_8^{(1)})^{-1}\hat{A})$	1.05	1.17	1.29	1.47	1.79
$k(\hat{A}^\top \hat{A})$	2.39e+3	2.65e+4	2.41e+5	1.79e+6	1.16e+7
$k(((P_8^{(1)})^\top P_8^{(1)})^{-1}\hat{A}^\top \hat{A})$	1.88	20.65	193.57	960.76	3.46e+3

the number of the temporal partition, respectively. In Tables 1 and 2, we present the average numbers of iterations, the errors computed by the sup-norm between the true solution and the numerical solution at the last time step and the CPU times (seconds) required by GMRES(20), PGMRES(20), CGNR, and PCGNR methods. We see that the number of iterations and execution time by the GMRES(20) and the CGNR methods increase dramatically, while those by the PGMRES(20) and PCGNR are changed little. The phenomena might be explained by the clustering of the eigenvalues of the relevant coefficient matrices. As an example, see Figure 1 for the distribution of eigenvalues of matrices  $\hat{A}$ ,  $\hat{A}^\top \hat{A}$ ,  $(P_8^{(1)})^{-1}\hat{A}$  and  $((P_8^{(1)})^\top P_8^{(1)})^{-1}\hat{A}^\top \hat{A}$  with  $m = n = 256$ . On the other hand, we see in Table 3 that the effect of the preconditioner on the condition numbers of the relevant matrices. The reader should be able to notice that the condition number significantly improves with the help of the proposed preconditioner.

## 5. Conclusion

Determining analytic solutions of FDEs is very challenging and remain unknown for most FDEs. This paper is to present an implicit approach to solve STFDE with two-sided Grünwald formulae. More significantly, with the aid of (15), we can ameliorate the calculation skill by the implementation of efficient and reliable preconditioning iterative techniques, the PGMRES method and the PCGNR method, with only computational cost of  $\mathcal{O}((m-1)\log(m-1))$ . Numerical results strongly suggest that the efficiency of the proposed preconditioning methods.

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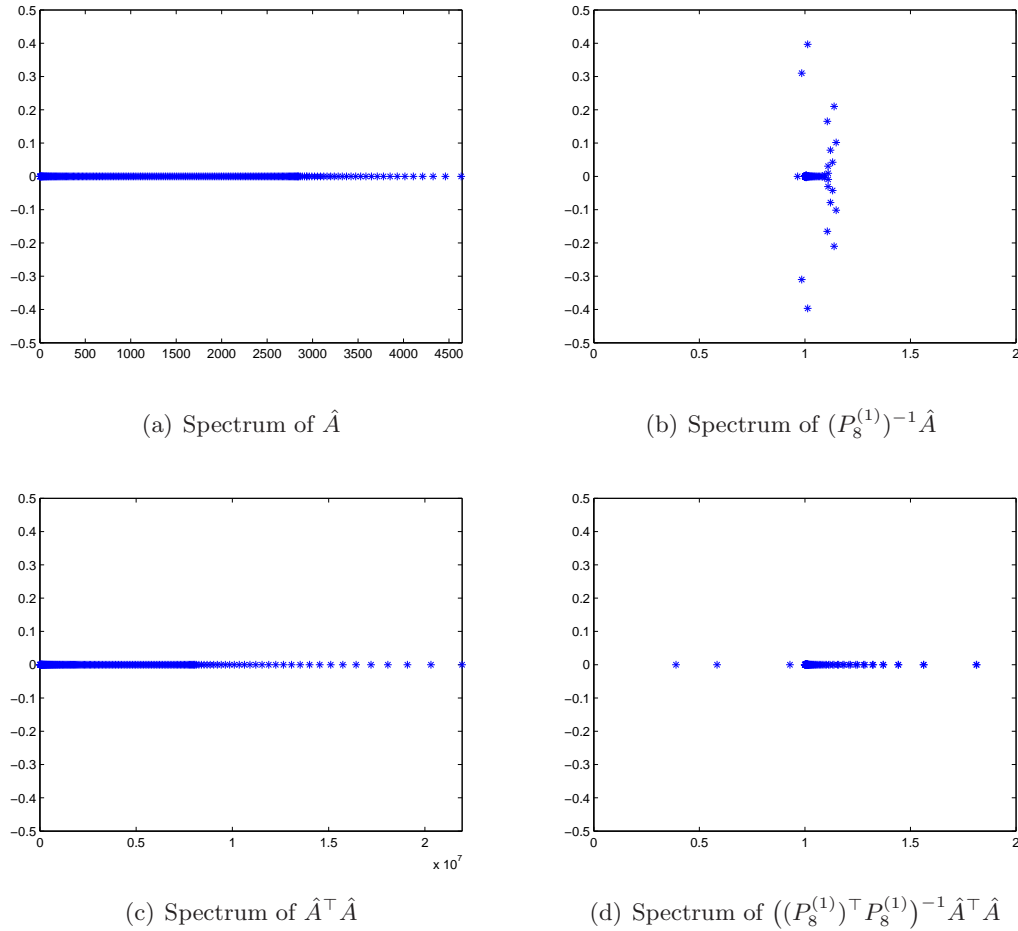


Figure 1: The Spectra of the unpreconditioned coefficient matrices and the preconditioned coefficient matrices with  $m = n = 256$ .

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